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***Abstract*—We propose a new smoothed ℓ_p-Over-ℓ_q norm ratio for sparse signal reconstruction. A trust-region Variable Metric Forward-Backward is proposed to solve efficiently the resulting non-convex minimization problem. Numerical experiments in the context of mass spectrometry (MS) illustrate the benefits of the novel penalty.**

I. Problem statement

We consider the linear observation model $\mathbf{y} = \boldsymbol{H}\mathbf{x} + \mathbf{n}$ where $\mathbf{y} = (y_m)_{1\leq m\leq M} \in \mathbb{R}^M$ represents the degraded measurements related to the original signal $\mathbf{x} = (x_n)_{1\leq n\leq N} \in \mathbb{R}^N$ through the observation matrix $\boldsymbol{H} \in \mathbb{R}^{M\times N}$ and some additive acquisition noise $\mathbf{n} \in \mathbb{R}^M$. In this work, we focus on the inverse problem aiming at recovering signal $\mathbf{x}$ from $\mathbf{y}$ and $\boldsymbol{H}$, under the assumption that the sought signal is sparse, *i.e.*, has few non-zero entries. An efficient strategy is to employ a penalized approach, which defines an estimate $\hat{\mathbf{x}} \in \mathbb{R}^N$ of $\mathbf{x}$ as the solution of the following constrained minimization problem

$$\underset{\mathbf{x}\in S}{\text{minimize}} \quad \Psi(\mathbf{x}) \quad \text{with} \quad S = \{\mathbf{x} \in \mathbb{R}^N \mid \|\boldsymbol{H}\mathbf{x} - \mathbf{y}\| \leq \xi\}. \tag{1}$$

Function $\Psi\colon \mathbb{R}^N \to]0, +\infty]$ is a regularization function used to enforce sparsity on the solution. Moreover, $\xi > 0$ is a parameter depending on the noise characteristics. The choice of the regularization function Ψ is important to reach satisfactory results.

II. Proposed approach

The ℓ_1 norm has probably been the most frequently used regularizer for sparse signal restoration. Special cases of quasi-norm ratios have also served as sparse penalities, for instance the ℓ_1/ℓ_2 ratio [1] or ℓ_4/ℓ_2 [2], with the advantage of limiting scale biases. In this work, we propose a new Smoothed p-Over-q (SPOQ) penalty defined as:

$$(\forall \mathbf{x} \in \mathbb{R}^N) \quad \Psi(\mathbf{x}) = \log\left(\frac{(\ell_{p,\alpha}^p(\mathbf{x}) + \beta^p)^{1/p}}{\ell_{q,\eta}(\mathbf{x})}\right), \tag{2}$$

where $p \in]0, 2[$ and $q \in [2, +\infty[$. We denote by $\ell_{p,\alpha}$ and $\ell_{q,\eta}$ the smoothed versions of ℓ_p and ℓ_q norms respectively given by $\ell_{p,\alpha}(\mathbf{x}) = \left(\sum_{n=1}^N \left(\left(x_n^2 + \alpha^2\right)^{p/2} - \alpha^p\right)\right)^{1/p}$ and $\ell_{q,\eta}(\mathbf{x}) = \left(\eta^q + \sum_{n=1}^N |x_n|^q\right)^{1/q}$ for every $\mathbf{x} \in \mathbb{R}^N$ and $(\alpha, \eta) \in]0, +\infty[^2$. In (2), the parameter $\beta \in]0, +\infty[$ is introduced to account for the fact that the log function is not defined at 0.

The SPOQ penalty is non-convex, which makes problem (1) challenging. It can however be shown that it is Lipschitz-differentiable on $\mathbb{R}^N$. Moreover, we established that Ψ presents a local majorization property. Let us define $\mathcal{B}_{q,\rho} = \{\mathbf{x} \in \mathbb{R}^N \mid \sum_{n=1}^N |x_n|^q \geq \rho^q\}$. Then, for every $(\mathbf{x}, \mathbf{x}') \in \mathcal{B}_{q,\rho}^2$, $\Psi(\mathbf{x}) \leq \Psi(\mathbf{x}') + \nabla\Psi(\mathbf{x}')^\top(\mathbf{x} - \mathbf{x}') + \frac{1}{2}(\mathbf{x} - \mathbf{x}')^\top \boldsymbol{A}_{q,\rho}(\mathbf{x}')(\mathbf{x} - \mathbf{x}')$ where, for every $\mathbf{x} \in \mathcal{B}_{q,\rho}$,

$$\boldsymbol{A}_{q,\rho}(\mathbf{x}) = \frac{1}{\ell_{p,\alpha}^p(\mathbf{x}) + \beta^p}\operatorname{Diag}\left((x_n^2 + \alpha^2)^{p/2-1}\right)_{1\leq n\leq N} + \frac{q-1}{(\eta^q + \rho^q)^{2/q}}\mathrm{I}_N.$$

We thus propose to solve (1) using the novel trust-region Variable Metric Forward Backward algorithm described below. It can be viewed as an extension of [3], where a trust-region strategy has been introduced in order to keep the iterates inside the sets fulfilling the majorization.

$\mathbf{x}_0 \in \mathbb{R}^N,\ B \in \mathbb{N}^*,\ \theta \in]0, 1[,\ (\gamma_k)_{k\in\mathbb{N}} \in]0, 2[$
For $k = 0, 1, \ldots$:
  For $i = 1, \ldots, B$:
    If $i = 1,\ \rho_{k,1} = \sum_{n=1}^N |x_{n,k}|^q$.
    If $i \in \{2, \ldots, B-1\},\ \rho_{k,i} = \theta\rho_{k,i-1}$.
    Else $\rho_{k,B} = 0$.
    Construct $\boldsymbol{A}_{k,i} = \boldsymbol{A}_{q,\rho_{k,i}}(\mathbf{x}_k)$
    $\mathbf{z}_{k,i} = \mathsf{P}_{\boldsymbol{A}_{k,i},S}\left(\mathbf{x}_k - \gamma_k(\boldsymbol{A}_{k,i})^{-1}\nabla\Psi(\mathbf{x}_k)\right)$
    If $\mathbf{z}_{k,i} \in \mathcal{B}_{q,\rho_{k,i}}$: Stop loop
  $\mathbf{x}_{k+1} = \mathbf{z}_{k,i}$

Hereabove, $\mathsf{P}_{\boldsymbol{A},S}$ denotes the projection onto S in the metric induced by $\boldsymbol{A}$ [3]. In this case, this projection cannot be explicitly expressed. We thus propose to compute it using the dual forward backward method [4]. Under mild assumptions, we proved that $(\mathbf{x}_k)_{k\in\mathbb{N}}$ converges to a critical point of Problem (1).

III. Application to mass spectrometry data analysis

We illustrate the usefulness of our proposed SPOQ penalty in the context of mass spectrometry (MS) data processing. MS is a fundamental technology of analytical chemistry widely used in structural biology [5], chemistry [6], pharmaceutical analysis [7], clinical drug development [8], etc. We have recently proposed a dictionary-based approach in [9] for proteins characterization in MS data. This method aimed at solving Problem (1) where Ψ is the ℓ_1 norm. We propose here to follow the same dictionary-based approach and to compare the results obtained by solving (1) using various choices of Ψ, namely the proposed SPOQ penalty for given p and q, the ℓ_1 norm, and the Cauchy and Welsh non-convex penalties [10].

Two synthetic signals A and B, with size $N = 1000$ and sparsity degree P are tested (Fig. 1 (top)). The associated MS spectra $\mathbf{y}$ are built with $\boldsymbol{H}$ being the MS averagine dictionary [11], and $\mathbf{n}$ a zero-mean Gaussian noise with standard deviation 10^{-2} (Fig. 1 (bottom)). Tab. I displays the means and standard deviations, on 10 noise realizations, for three metrics: SNR= $20\log_{10}(\|\mathbf{x}\|/\|\mathbf{x} - \hat{\mathbf{x}}\|)$, TSNR defined as the SNR computed only on the support of the sought sparse signal, and sparsity, i.e. the number of entries of the restored signals greater (in absolute value) than a given threshold (here, 10^{-4}). We can observe that SPOQ is superior to the three other penalties with respect to all metrics. In particular, $p = 0.25$ and $q = 2$ seem to provide an optimal choice in terms of estimation accuracy.

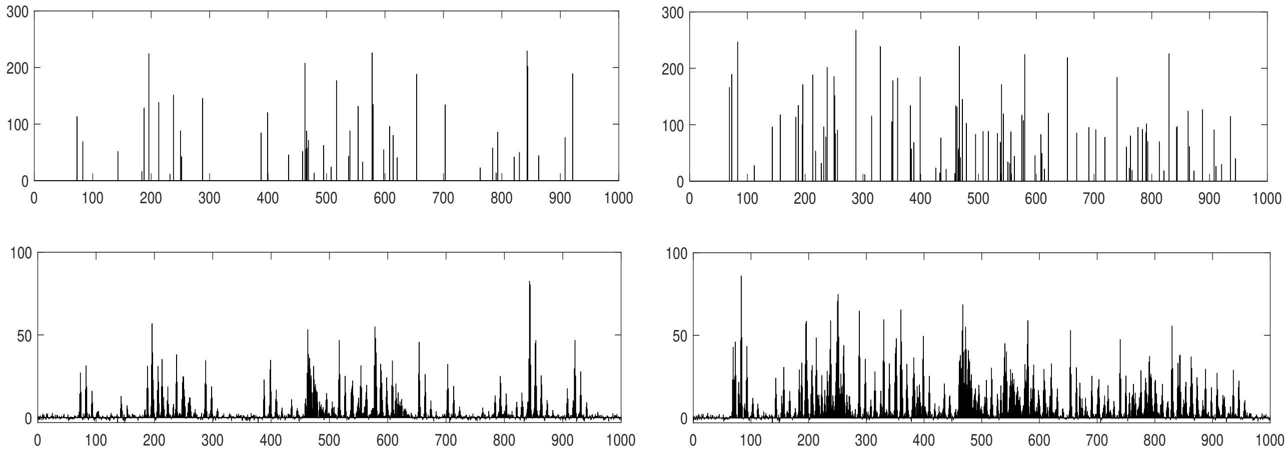

Figure 1. Original sparse signals and associated MS spectra for dataset A (left, $N = 1000$, $P = 48$) and dataset B (right, $N = 1000$, $P = 94$) (top: synthetic data, bottom: noisy MS spectra).

		P	$\ell_{0.25}/\ell_2$	$\ell_{0.5}/\ell_2$	ℓ_1/ℓ_2	ℓ_1	Cauchy	Welsh
Signal A	SNR	48	**46.28**	41.91	40.91	43.16	42.84	27.54
			0.497	*0.436*	*0.910*	*0.654*	*0.572*	*0.461*
	TSNR	48	46.55	**47.71**	46.24	43.94	43.53	29.12
			0.571	*1.136*	*1.660*	*0.679*	*0.532*	*0.501*
	Sparsity	48	**49**	129	365	80	883	259
			1.32	*11.85*	*10.13*	*9.46*	*10.57*	*8.08*
Signal B	SNR	94	**45.56**	42.74	41.31	43.02	42.71	30.99
			0.538	*1.266*	*1.298*	*1.260*	*1.194*	*0.488*
	TSNR	94	**47.26**	46.88	45.11	44.17	43.68	33.39
			0.639	*1.495*	*1.654*	*1.138*	*0.961*	*0.507*
	Sparsity	94	**111**	216	410	165	952	342
			3.54	*12.43*	*11.03*	*17.41*	*6.66*	*11.72*

Table I

MEANS/STDS OF SNR, TRUNCATED SNR AND SPARSITY LEVEL OF THE RESTORED SIGNALS. COMPUTED ON 10 NOISE REALIZATIONS FOR DATASETS A AND B AND VARIOUS PENALTIES.

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REFERENCES

[1] A. Repetti and M. Q. Pham and L. Duval, E. Chouzenoux and J.-C. Pesquet. *Euclid in a Taxicab: Sparse Blind Deconvolution with Smoothed ℓ_1/ℓ_2 Regularization* IEEE Signal Processing Letters, Vol. 22, No 5, pages 539–543, May 2015,

[2] R. A. Wiggins, *Minimum entropy deconvolution*, Proc Int. Symp. Computer Aided Seismic Analysis and Discrimination, pages 7–14, Jun. 1977.

[1]https://www.i2m.univ-amu.fr/project/bifrost

[2]http://www-syscom.univ-mlv.fr/∼chouzeno/MajIC

[3] E. Chouzenoux, J.-C. Pesquet and A. Repetti. *Variable Metric Forward-Backward Algorithm for Minimizing the Sum of a Differentiable Function and a Convex Function*, Journal of Optimization Theory and Applications, Vol. 162, No. 1, pages 107–132, Jul. 2014.

[4] F. Abboud, E. Chouzenoux, J. C. Pesquet, J. H. Chenot and L. Laborelli, *Dual block-coordinate forward-backward algorithm with application to deconvolution and deinterlacing of video sequences*, Journal of Mathematical Imaging and Vision, volume 59, no. 3, pages 415–431, 2017.

[5] L. M. Heaney, D. J. Jones, and T. Suzuki, *"Mass spectrometry in medicine: a technology for the future?,"* Future Science OA, vol. 3, no. 3, June 2017.

[6] I.-E. Sodal, *The medical mass spectrometer*, Biomedical Instrumentation and Technology, vol. 23, no. 6, pages. 469–476, 1989.

[7] P. Mira, H. Maria, D. Cruz, M. Silva, B. Damia. *Liquid chromatography-tandem mass spectrometry for the analysis of pharmaceutical residues in environmental samples*, Journal of Chromatography A, vol. 1067, no. 1-2, pages. 1–14, 2005, Springer.

[8] P.-J., James. *Principles and applications of liquid chromatography-mass spectrometry in clinical biochemistry*, The Clinical Biochemist Reviews, vol. 30, no. 1, pages 19, 2009.

[9] A. Cherni, E. Chouzenoux and M.-A. Delsuc. *Fast Dictionary-Based Approach for Mass Spectrometry Data Analysis*, In Proceedings of the IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP 2018), Calgary, Canada, 15-20 April 2018.

[10] E. Chouzenoux, A. Jezierska, J.-C. Pesquet and H. Talbot. *A Majorize-Minimize Subspace Approach for l2-l0 Image Regularization*, SIAM Journal on Imaging Science, Vol. 6, No. 1, pages 563–591, 2013.

[11] M.-S. Senko, J. Paul, M.-W. Fred. *Collisional activation of large multiply charged ions using Fourier transform mass spectrometry*, Analytical Chemistry, vol. 66, no. 18, pages 2801–2808, 1994.